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4-(3,4-Dimethyl-5-phenyl-1,3-oxazolidin-2-yl)-2-methoxyphenol

Mohd Razip Asaruddin,[a] Habibah A Wahab,[b]‡ Nornisah Mohamed,[a] Jia Hao Goh[c]§ and Hoong-Kun Fun[c]*¶

[a]Pharmaceutical Design and Simulation Laboratory, School of Pharmaceutical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Institute of Pharmaceutical and Neutraceuticals, Malaysia Ministry of Science and Technology and Innovation, Science Complex, 11900, Penang, Malaysia, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

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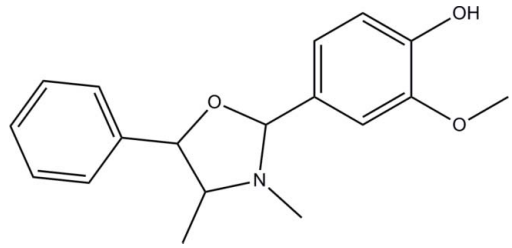
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.096; data-to-parameter ratio = 10.3.

In the title compound, $C_{18}H_{21}NO_3$, the oxazolidine ring adopts an envelope conformation with the N atom at the flap position. The two benzene rings make dihedral angles of 74.27 (14) and 73.26 (15)° with the mean plane through the oxazolidine ring. In the crystal structure, O—H···O and C—H···O hydrogen bonds connect adjacent molecules into chains along [010] incorporating $R_2^2(8)$ loops and further stabilization is provided by weak intermolecular C—H···π interactions.

Related literature

For general background to and applications of the title oxazolidine compound, see: Fitzgerald *et al.* (2005); Kamat *et al.* (2000); Kumar *et al.* (2004); Walton *et al.* (2003). For graph-set descriptions of hydrogen-bond ring motifs, see: Bernstein *et al.* (1995). For a related structure, see: Duffy *et al.* (2004). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{18}H_{21}NO_3$
M_r = 299.36
Orthorhombic, $P2_12_12_1$
a = 7.8893 (6) Å
b = 11.7697 (9) Å
c = 17.4392 (13) Å
V = 1619.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 120 K
0.31 × 0.15 × 0.15 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.975, T_{max} = 0.987
9140 measured reflections
2131 independent reflections
1622 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.096
S = 1.07
2131 reflections
206 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C10–C15 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*1···O3^{i}	0.92 (4)	2.08 (3)	2.909 (3)	148 (3)
C5—H5*A*···O1^{ii}	0.93	2.42	3.244 (3)	148
C16—H16*A*···*Cg*1^{iii}	0.96	2.91	3.628 (3)	133

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y-1, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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‡ Additional correspondence author, e-mail: habibahw@usm.my, habibah@ipharm.gov.my. On secondment from: Pharmaceutical Design and Simulation Laboratory, School of Pharmaceutical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia.
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